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Ab initio calculation of the electronic structure of Fe and Cr interlayers

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The band structure, diversity of structure and various band gaps have been calculated using ab initio density functional theory (DFT) for some interlayer structures consisting of Fe and Cr atoms, viz. (a) Fe-Cr, (b) Fe-Fe-Cr-Cr and (c) Fe-Fe-Cr-Cr-Fe-Fe-Cr-Cr. Calculations have been done for spin-polarized as well as unpolarized orbitals. The spins are shown to affect the band gaps and resistivity considerably. As a test, we also obtained the band structure of Fe and Cr bulk unit cells. An effort is made to discuss the resistivity as a function of spin.

Keywords: Fe-Cr interlayers; band structure; magnetoresistance

Introduction

The electron energy bands in periodic lattices pose a considerably long problem in terms of the size of the secular determinant. A small 2×2 determinant shows that there are bands and gaps in the eigen values of electrons in a periodic potential. The number of electrons per atom and the number of atoms in a unit cell determine the size of the secular determinant which can be solved by means of a high speed modern computer by using approximations such as the local density approximation (LDA) or the generalized gradient approximation. In the case of single crystals, the electron energies can be obtained at various points of the Brillouin zone. In the modern times, the emphasis has been laid on layers of atoms, multilayers and tubes. In a sample of Fe film of about 12 nm thickness, a layer of Cr atoms of thickness 1 nm is deposited and then another layer of Fe atoms of about 12 nm thickness is deposited so as to form three films one over the others, Fe-Cr-Fe, of thickness of about 25 nm. This device has special properties. When external field is zero, the magnetization in the two layers is opposite to that in each other. When a magnetic field is applied the moments in each film of Fe atoms align parallel to each other. It turns out that in zero field, when the magnetization in the two films is oppositely directed, the resistivity is very large. When magnetic field of about 1000 Gauss is applied, the moments in the two films of Fe become parallel and the resistivity becomes very small. This is the phenomenon of magnetoresistance[1,2]. The direction of magnetization depends on the orientation of the crystallographic axes. In thin films of thickness of about 12 nm, the magnetization is directed along ^{100} direction. For small thickness, the direction of the magnetic moment is along ^{110} direction which shows that there is anisotropy which depends on the crystallographic orientation. In the case of 25 nm thick Fe films, the magnetic field required to align the magnetization in the two films is about 1500 Gauss at which the resistivity becomes very small. At the zero field, 25 nm thick Fe with Cr and again Fe film device, the resistivity is about 15 per cent higher in antiparallel configuration than in parallel system. Therefore, there is clearly a large change in the resistivity between the parallel and the antiparallel magnetization samples. In the case of layered samples, the setting up of the hamiltonian has been described by Buchmeier *et al*[3]. It requires a coordinate transformation. There is a very strong ``AF interlayer" exchange coupling of ~6 mJ/m^2 in Fe/Si/Fe trilayer system. Gareev *et al*[4] have measured the antiferromagnetic exchange interaction between Fe atoms for varying thickness of Si spacers. They are able to measure the biquadratic exchange interaction $j(S_i.S_j)^2$. It may be recalled that repulsive Coulomb interactions give rise to ferromagnetism whereas the electron-nuclear attractive potential introduces antiferromagnetism. The biquadratic interaction permits a phase transition from the ferromagnetic to antiferromagnetic configuration. It is also believed that the biquadratic exchange interaction gives rise to magnetostriction[5]. The application of Boltzmann's transport equation to the Fe/Cr layered structure has been described by Camley and Barnas[6].

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Introduction

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110

In Co/Au/Co also, the usual ferromagnetic cobalt aligns antiparallel when Au film is introduced in between[7]. Katine *et al*[8] suggest that electrons flow from one layer to the other and reverse spin due to the potential. Similar results for Co/Ru/Co have been obtained[9-13]. The antiferromagnetic interactions in Fe/Cu/Fe and Co/Cu/Co have also been reported[14]. The magnetization alignment is due to the potential. In recent years, we have developed the density-functional theory calculations of correlation energies and vibrational frequencies from the first principles which are in reasonable agreement with the experimental data[15-18]. The ab initio calculations are known to yield results which are useful for the understanding of electron energies[19-21].

In this letter, we use the density-functional theory to make the models of a single layer of Fe over a single layer of Cr, Fe-Cr, 2 layers of Fe over two layers of Cr, Fe-Fe-Cr-Cr and alternately two layers of Fe, two layers of Cr, two layers of Fe and again two layers of Cr, Fe-Fe-Cr-Cr-Fe-Fe-Cr-Cr. In each case, we have calculated the density of states and the band structure. We are able to find the electron energy states which may be relevant to the understanding of the interlayer systems. We also discuss the resistivity changes due to spin.

Methodology

Large secular determinants are solved by using the density-functional theory. The two approximations, the local density approximation (LDA) and the generalized gradient approximation (GGA) are most commonly used. The idea is to break down the Schroedinger equation into Kohn-Sham equations which make the problem tractable. There are two approaches to solve this problem. The computer program called the CASTEP was developed in Cambridge, U.K. and is now available in the modern graphics interface. This programme uses the pseudopotentials which replace some of the core electrons. Another programme is called the DMol^3 which uses all of the electrons without any pseudopotentials. The programmes are available from the Accelrys Software Inc, Sandiego, Ca. The present calculations are done by using DMol^3 on a quadro computer. In another paper, we will show the differences in the values obtained by using different programmes.

Band structure calculations

The band energy levels of body-centred cubic (b.c.c.) Fe are given by Tawil and Callaway[22]. The Γ points are located in the centre of the Brillouin zone. The H points are on the corners of a face and N points are on the face centres. For pure Fe, the energies at the various points are given in Table 1. We have also included the values calculated by Wakoh and Yamashita[23], Duff and Das[24] and Woodruff[25] along with our values. It is found that our values calculated by using the DFT are reasonably close to those given by Tawil and Callaway[22]. The agreement between our values and those of Callaway serves as a test of our calculations. We also calculated the band structures of several elements, such as diamond, to find that our computer program works well. We have calculated the band structure of iron with spin-polarized orbitals as well as without polarization. In the case of unpolarized calculations the bands start near zero energy at G point whereas in the polarized case, this point is slightly raised up by about 0.06 Hartree [1 Hartree= 27.211 3845(23) eV]. Thus we see that spin polarization plays an important role in determining the energies. The density of states (DOS) of Fe for the spin polarized orbitals is calculated. The DOS of d orbitals is peaked and concentrated near zero energy, whereas that of s orbitals is much smaller than that of d orbitals. This means that the magnetism in Fe is due to the d orbitals.

We have calculated the band structure of Cr by using unpolarized orbitals. The calculated values of the band gap energies are given in Table 2 along with those calculated by Asano and Yamashita[26], Gupta and Sinha[27], Yasui *et al*[28] and Rath and Callaway[29]. Our values are in reasonable agreement with those of other authors. The DOS clearly shows that d electrons are localized and represent a much larger fraction than s electrons.

4. Band structure of interlayers

One layer of Fe with one layer of Cr(Fe-Cr=1,1 layer), are made according to the primitive cells. The calculated values of the cell constants are a=b=2.4899 Å and c=6.2462 Å. In this case, the Fermi energy is 7.95 eV and binding energy is 14.77 eV for spin-polarized wave functions and Fermi energy is 7.93 eV with binding energy of 13.65 eV for

unpolarized wave functions. The unpolarized band structure is shown in Fig. 1 and the polarized band structure is given in Fig.2. The Fermi energy, given in Table 3, shows only a small variation as a function of layered structure. The DOS with polarized orbitals is given in Fig. 3. There is the usual localization near zero energy but there is a broad peak at slightly higher energies. The spin level doubling in the polarized case is clearly visible.

Table 1– The band gaps of Fe calculated at various points in eV.

Zone points	Ref.22	Ref.23	Ref.24	Ref.25	This work
$(H_{12}-H_{25})\uparrow$	4.4899	4.7620	10.0682	---	4.6805
$(H_{12}-H_{25})\downarrow$	5.0341	5.3062	---	5.9865	5.1159
$(\Gamma_1-\Gamma_{25})\uparrow$	4.7620	5.4423	7.8913	---	6.0139
$(\Gamma_1-\Gamma_{25})\downarrow$	5.9865	6.6668	---	4.4899	7.4833
$(\Gamma_{12}-\Gamma_{25})\uparrow$	1.7687	1.4966	3.1293	---	1.3606
$(\Gamma_{12}-\Gamma_{25})\downarrow$	1.9048	1.4966	---	1.6327	2.0409
$(P_4-P_3)\uparrow$	2.8572	2.4490	6.1226	---	2.5851
$(P_4-H_3)\downarrow$	3.4014	2.9933	---	3.4014	3.6736

Table 2– The gap energies of Cr calculated at various points in eV by using unpolarized orbitals.

Zone points	Ref.26	Ref.27	Ref.28	Ref.29	This work
$\Gamma_{12}-\Gamma_1$	7.8709	9.6464	7.7416	8.3022	8.8439
$\Gamma_{12}-\Gamma_{25'}$	1.8123	1.8504	1.9728	2.1633	2.1770
$\Gamma_{25'}-\Gamma_1$	6.0573	7.7961	5.7688	6.1402	6.6669
$H_{25'}-H_{12}$	6.5960	7.1158	6.3539	6.5471	6.2588
$H_{15}-\Gamma_1$	---	18.0956	14.9254	17.2030	18.1640
$H_{25'}-\Gamma_{25'}$	3.1851	3.2382	4.0545	3.6327	3.2654
$\Gamma_{12}-H_{25}$	5.2246	5.7280	4.2722	5.0749	5.3063
P_3-P_4	3.4082	4.0817	3.0885	3.6327	4.0818
N_2-N_1	1.8041	2.3130	1.4830	1.6789	1.8232
N_3-N_1	6.8369	7.5920	6.7756	7.2137	6.8574
N_4-N_1	0.2721	---	---	0.2871	0.1088
$N_{1'}-N_4$	0.7211	---	---	0.1565	0.4626
$N_3-N_{1'}$	0.6776	---	0.9388	1.4789	0.9252

Table 3. The Fermi energy and the binding energy in eV.(unpol=unpolarized, pol.=polarized) (present work).

Energy	Fe-Cr unpol	Fe-Cr pol	Fe(2)-Cr(2) unpol	Fe(2)-Cr(2) pol	Fe(2)-Cr(2)-Fe(2)-Cr(2) unpol	Fe(2)-Cr(2)-Fe(2)-Cr(2) pol
Fermi	9.93	7.95	7.94	7.93	7.91	7.80
Binding	13.65	14.77	54.81	57.35	23.05	24.98

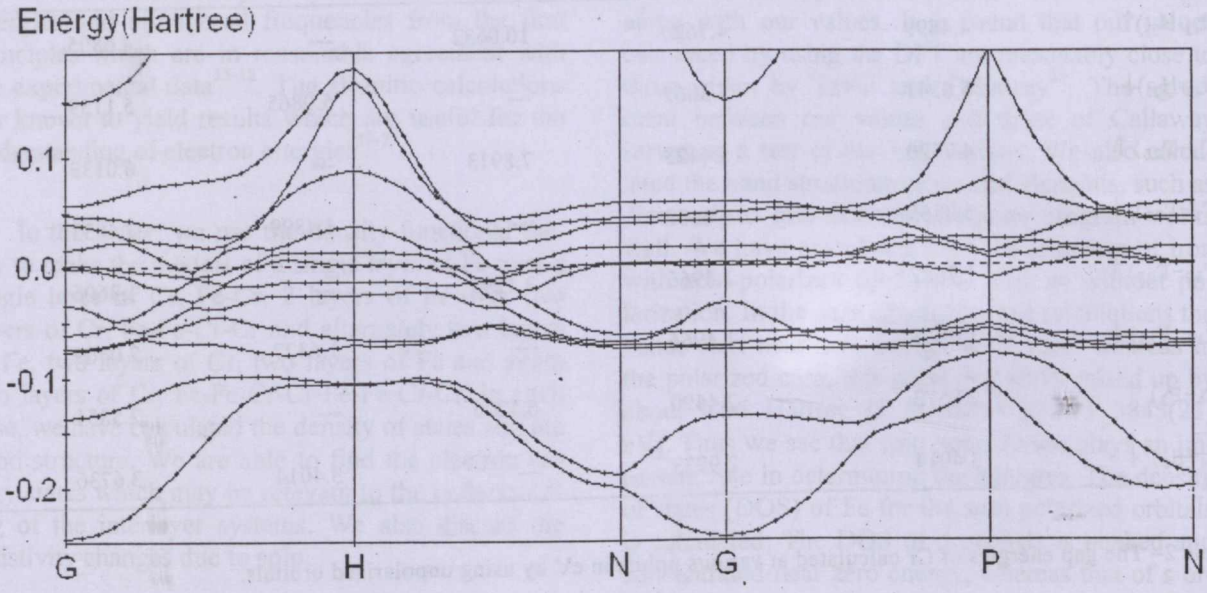

Fig. 1– The band structure of a mono-atomic layer of Fe over a mono-atomic layer of Cr with unpolarized orbitals.

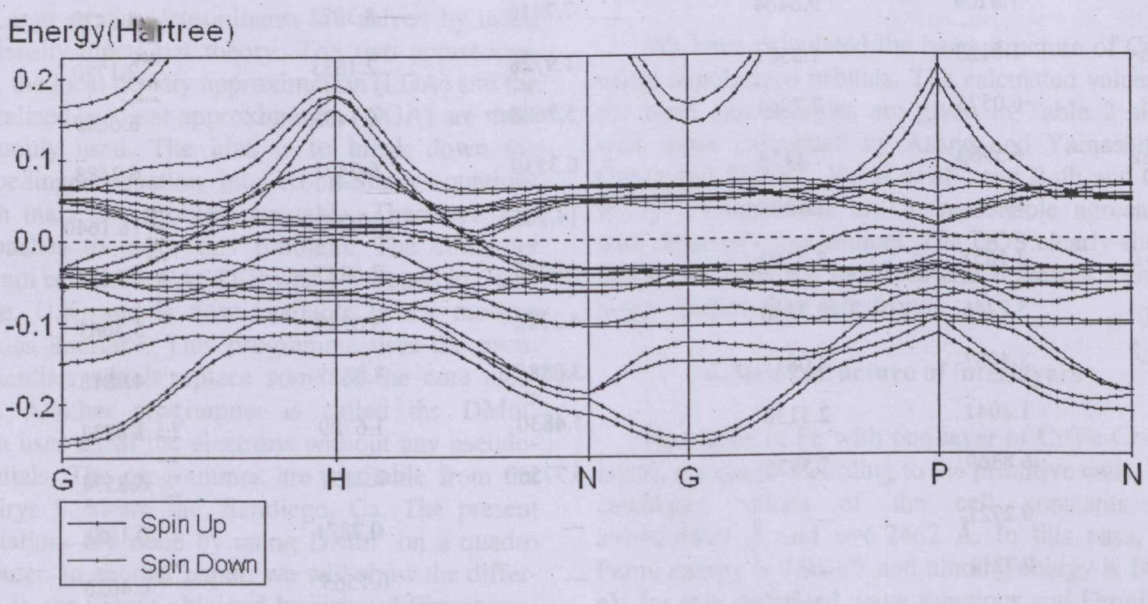

Fig. 2– The band structure of monoatomic layer of Fe over mono-atomic layer of Cr with polarized orbitals.

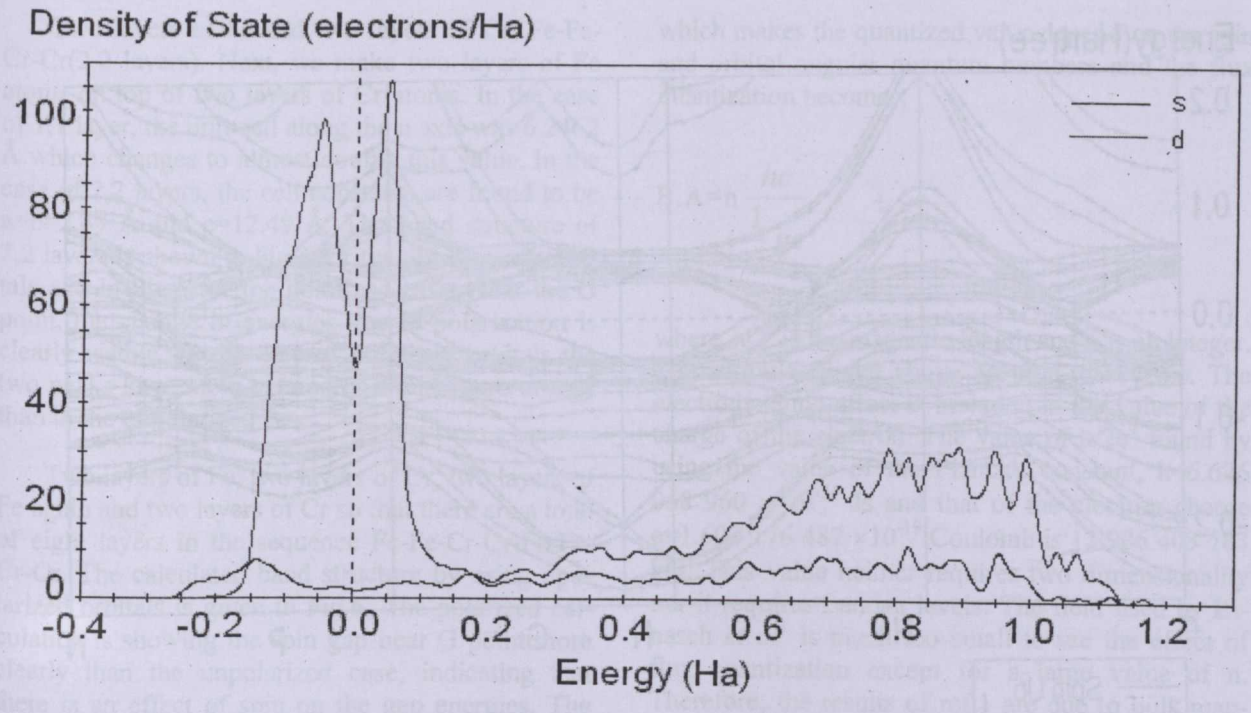

Fig. 3– The DOS of FeCr with spin-unpolarized orbitals.

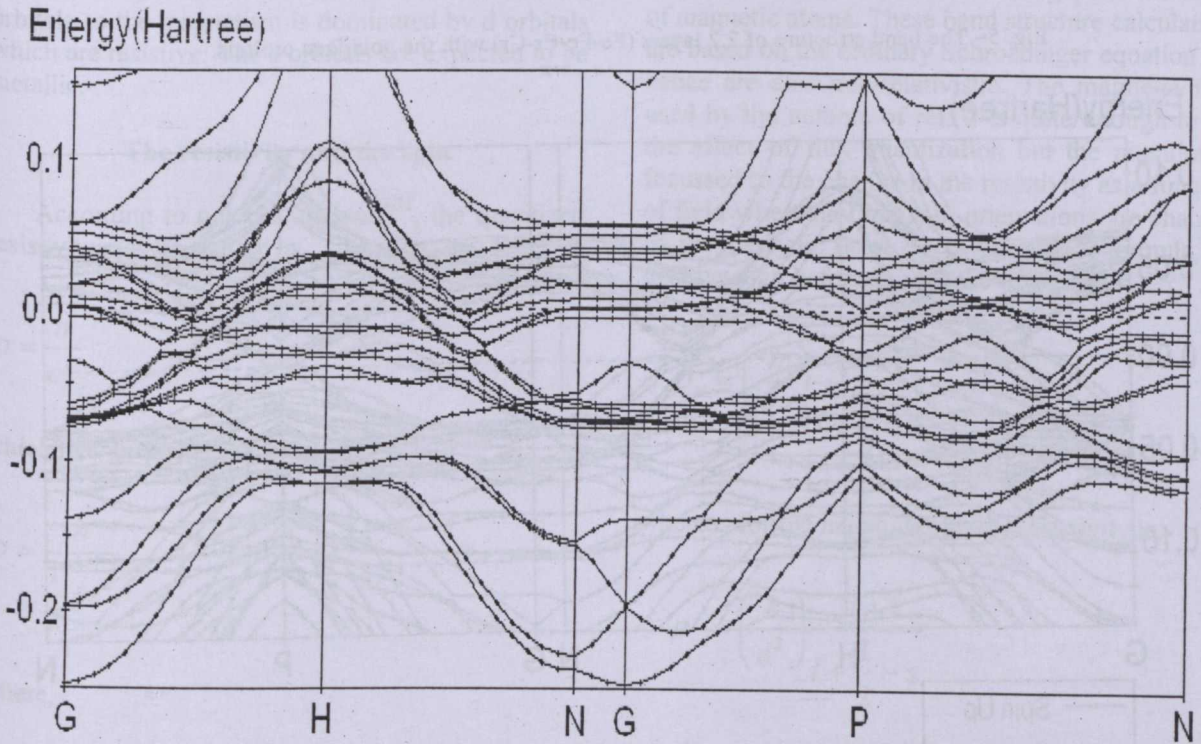

Fig. 4– The band structure of 2,2 layers (Fe-Fe-Cr-Cr) with the unpolarized orbitals.

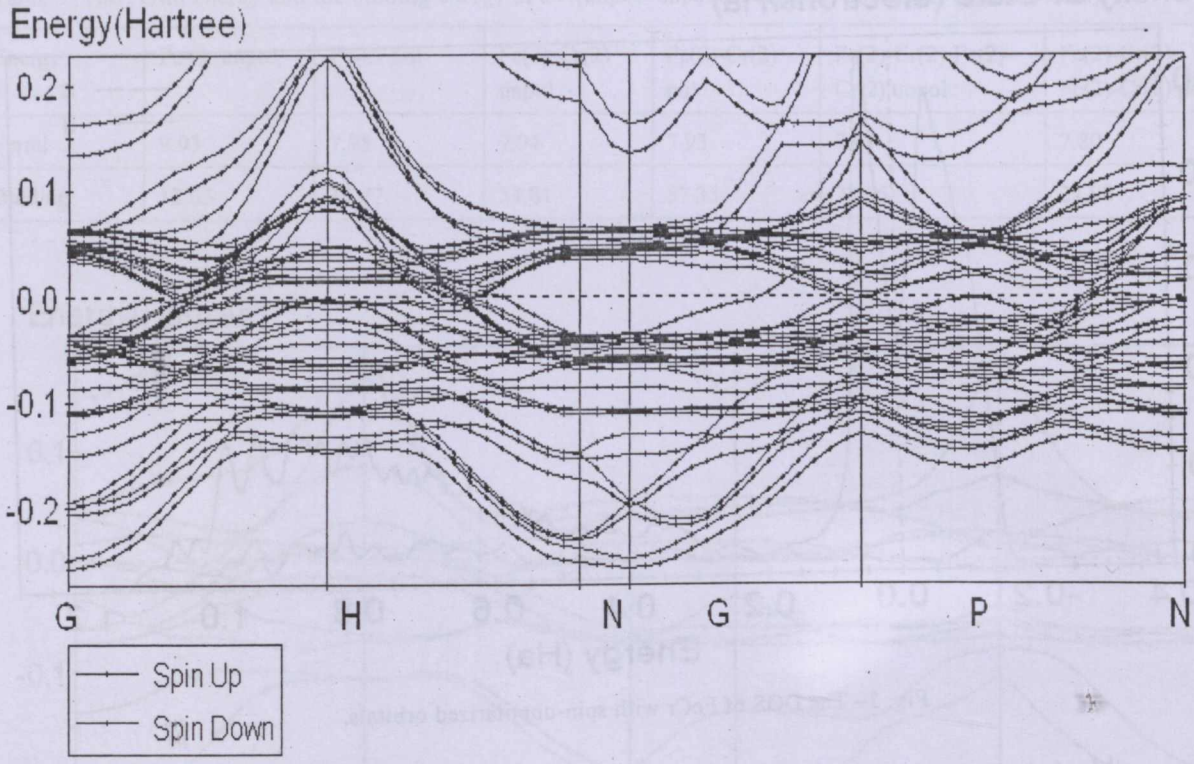

Fig. 5– The band structure of 2,2 layers (Fe-Fe-Cr-Cr) with the polarized orbitals.

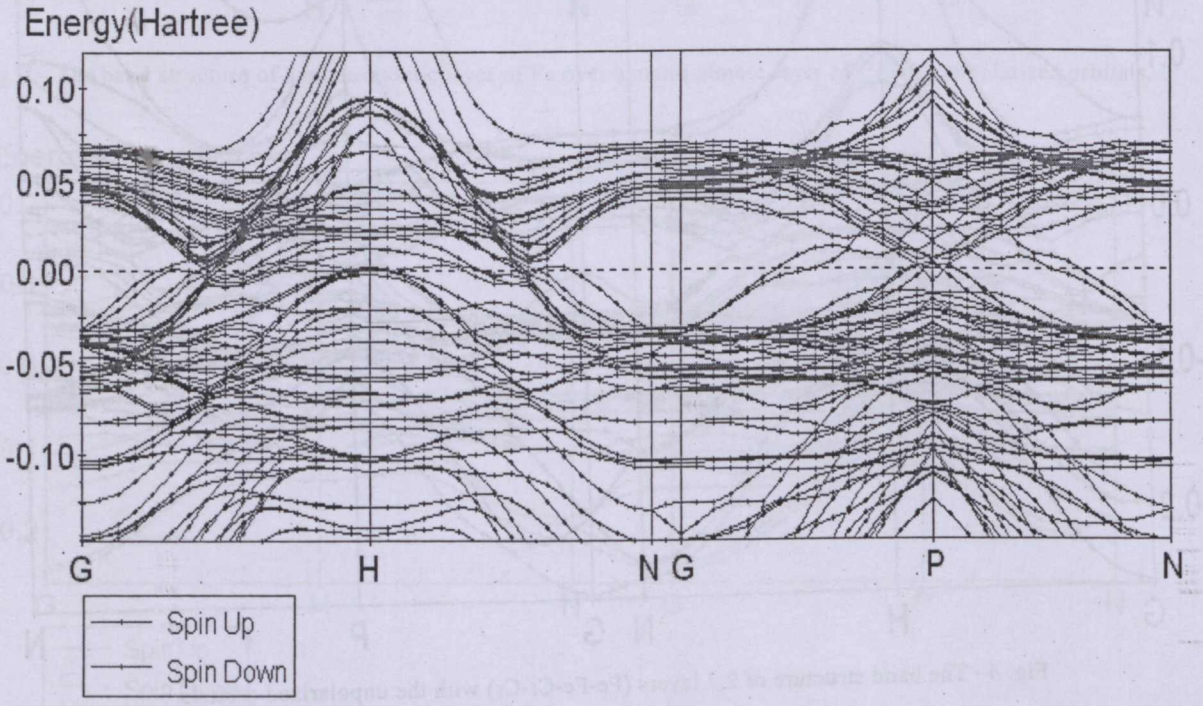

Fig. 6– The band structure of eight layers, Fe-Fe-Cr-Cr-Fe-Fe-Cr-Cr with polarized orbitals.

Two layers of Fe and two layers of Cr, Fe-Fe-Cr-Cr(2,2 layers). Next, we make two layers of Fe atoms on top of two layers of Cr atoms. In the case of 1,1 layer, the unit cell along the c axis was 6.2462 Å which changes to almost double this value. In the case of 2,2 layers, the cell constants are found to be a=b=2.49 Å and c=12.49 Å. The band structure of 2,2 layers is shown in Fig.4 for the unpolarized orbitals and in Fig.5 for the polarized case. Near the G point, the change in energies due to polarization is clearly visible. In the case of polarized orbitals the two peaks have more symmetry around zero energy than in the unpolarized case.

Two layers of Fe, two layers of Cr, two layers of Fe again and two layers of Cr so that there are a total of eight layers in the sequence Fe-Fe-Cr-Cr-Fe-Fe-Cr-Cr. The calculated band structure by using upolarized orbitals is given in Fig.6. The polarized calculation is showing the spin gap near G point more clearly than the unpolarized case, indicating that there is an effect of spin on the gap energies. The DOS of this system shows that most of the density is in d orbitals and much smaller value is seen in the s orbitals so the magnetism is dominated by d orbitals which are resistive. The s orbitals are expected to be metallic.

The resistivity and the spin

According to our calculation[30-31], the quantized resistivity may be written as,

$$\rho = \frac{h}{e^2}$$

which may be corrected to,

$$\rho = \frac{h}{\frac{1}{2} g e^2}$$

where,

$$\frac{1}{2} g = \frac{l + \frac{1}{2} \pm s}{2l+1}$$

which makes the quantized value depend on the spin and orbital angular quantum numbers and the flux quantization becomes,

$$B.A = n \frac{hc}{\frac{1}{2} ge}$$

where $A^{1/2}$ is the magnetic length and n is an integer. The formulas given above are non-relativistic. The electrodynamic effect is included in the value of the charge of the electron. The value of $h/2e^2$ found by using the value of the Planck's constant, h=6.626 068 960 × 10^{-34} Js and that of the electron charge e=1.602 176 487 ×10^{-19} Coulomb is 12.906 403 783 kΩ. This value neither requires two dimensionality nor it requires Landau levels. The field used by Binasch *et al*[1] is much too small to see the effect of flux quantization except for a large value of n. Therefore, the results of ref.1 are due to bulk magnetization. From the band structure calculations we learn that there are spin dependent gaps in the layers of magnetic atoms. These band structure calculations are based on the ordinary Schroedinger equation and hence are also non-relativistic. The magnetic field used by the authors of ref. 2 is quite enough to see the effect of flux quantization but the attention is focussed to the change in the resistivity as a function of field when the bulk spin orientations are changed by the magnetic field. According to our formula, the positive sign before s gives the resistivity,

$$\rho_+ = \left(\frac{h}{e^2}\right) \frac{2l+1}{l + \frac{1}{2} + s}$$

whereas for the negative sign the resistivity is,

$$\rho_- = \left(\frac{h}{e^2}\right) \frac{2l+1}{l + \frac{1}{2} - s}$$

For l =0, s=1/2, $\rho_+ = \frac{h}{e^2}$ and $\rho_- = \infty$. Therefore, large changes in the resistivity are possible when the

sign of the spin is changed. The above values suggest change in resistivity from 25.8 kΩ to unity upon spin flip. If we substitute i=0, then the resistivity changes from 2.5 kΩ to infinity. Of course there are other values which show the resistivity as a function of spin. We need not limit to s=1/2 only. Other values of the spin such as 3/2 or 5/2 are also allowed.

Conclusions

We have performed the ab initio calculations for the band structure of Fe-Cr mono-atomic layers. We have also performed the band structure calculations for two layers of Fe over two layers of Cr and also for the eight layer system, Fe-Fe-Cr-Cr-Fe-Fe-Cr-Cr for spin polarized as well as unpolarized orbits. We find that there is considerable effect of spin on the band gaps. We also find that resistivity depends on spin. These theoretical results will serve as prototype models for the understanding of bulk magnetization and the resistivity.

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